ISOTHERMAL VAPOR-LIQUID EQUILIBRIA OF CYCLIC DIETHERS WITH HEXANE, CYCLOHEXANE OR ETHANOL

[a]Encina Calvo, [a]Ramón Bravo, [b]Carmen Jarne, [b]Manuela Artal

[a]Departamento de Física Aplicada, Facultad de Física, Universidad de Santiago, 15706-Santiago de Compostela, Spain
[b]Departamento de Química Orgánica-Química Física, Facultad de Ciencias, Universidad de Zaragoza, 50009-Zaragoza, Spain

This work forms part of a program to determine excess thermodynamic properties for a number of binary and ternary mixtures involving {a cyclic ether + a polar or non-polar solvent}. In earlier papers [1-2] we have reported the results for measurements of excess volumes, excess enthalpies and excess molar heat capacities of mixtures of cyclic ethers with alkanes or alkanols. The aim if these investigations was to correlate the experimental data with different factors affecting interactions between components in such mixtures. As an extension of those studies, the present work reports the isothermal vapor-liquid equilibria for liquid 1,4-dioxane or 1,3-dioxolane + n-hexane, cyclohexane or ethanol at the temperature 298.15 K.

Vapor-liquid equilibrium data were taken at constant temperature in a dynamic still designed by Berro et al. [3]. The temperature inside the equilibrium cell was measured with a precision of 0.01 K by a Digitec digital thermometer (Digitel Corp., Model 5831). The pressure P was measured by a Digiquartz Transmitter (Paroscientific Inc., Model 1015A) calibrated in the pressure range 0-0.1 Mpa. The accuracy of the pressure measurements is 0.01%. Liquid and vapor mole fractions, x_1 and y_1, respectively, were determined by densimetric analysis using an Anton Paar Model DMA 60 densimeter equipped with a DMA 602 cell in a flow system as described by Muñoz Embid et al. [4].

On the other hand, group contribution theories such as Nitta-Chao, Uniquac, Unifac or Disquac have been used to calculate thermodynamic properties (G^E, H^E, C_p^E, ...) and to determine the temperature dependence of the VLE. Such information is needed by industry to optimise processes or to replace toxic or dangerous solvents by mixtures offering grater safety. The VLE data reported in this work have been used to calculate the characteristic parameters of the Nitta-Chao group contribution model corresponding to the cyclic ethers, and the predictions of this model have been compared with the experimental results.

[1] E. Calvo, P. Brocos, R. Bravo, M. Pintos, A. Amigo, A.H. Roux and G. Roux-Desgranges, *J. Chem. Eng. Data*, **43**, 105 (1997).
[2] E. Calvo, P. Brocos, R. Bravo, M. Pintos, A. Amigo, A.H. Roux and G. Roux-Desgranges, *J. Chem. Eng. Data*, **43**, 112 (1997).
[3] C. Berro, M. Rogalski and A. Péneloux, *Fluid Phase Equilibria*, **8**, 55 (1982).
[4] J. Muñoz-Embid, M. Artal, J. Fernández, I. Velasco and S. Otín, *J. Chem. Eng. Data*, **36**, 428 (1991).